

Quantum ripples in strongly correlated metals

E. C. Andrade,^{1,2} E. Miranda,¹ and V. Dobrosavljević²

¹*Instituto de Física Gleb Wataghin, Unicamp, C.P. 6165, Campinas, SP 13083-970, Brazil*

²*Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306*

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We study how well-known effects of the long-ranged Friedel oscillations are affected by strong electronic correlations. We first show that their range and amplitude are significantly suppressed in strongly renormalized Fermi liquids. We then investigate the interplay of elastic and inelastic scattering in the presence of these oscillations. In the singular case of two-dimensional systems, we show how the anomalous ballistic scattering rate is confined to a very restricted temperature range even for moderate correlations. In general, our analytical results indicate that a prominent role of Friedel oscillations is relegated to weakly interacting systems.

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Introduction.—Fermi liquid theory is known to successfully describe the leading low temperature behavior of metals, even in instances of very strong correlations (e.g. heavy fermions [1]). In the presence of perturbations that break translational symmetry, such as impurities and defects, the Fermi liquid re-adjusts itself producing a spatially inhomogeneous pseudo-potential “seen” by quasiparticles [2, 3]. Here the wave nature of the electrons is manifested by the formation of “ripples”, the Friedel oscillations [4, 5], surrounding the perturbation. Scattering processes of quasiparticles off these ripples then produce new corrections to the T -dependence in transport quantities [6].

How significant are these corrections? The answer, of course, depends on how broad the dynamic range is, in which such leading order non-analyticities dominate. This question, as usual, cannot be answered by Fermi liquid theory itself. What is needed is a microscopic model calculation that is not restricted to obtaining the form of leading terms. A careful and precise model calculation with such a goal is the central content of this paper.

We focus on single non-magnetic impurity scattering in an otherwise uniform strongly interacting paramagnetic metal, where the analysis is most straightforward and transparent, but this general issue is of key relevance also for the diffusive regime. Our mostly analytical results demonstrate that: (i) for sufficiently weak correlations we recover the results of the Hartree-Fock approximation, in which the effective scattering potential generated by the impurity is set by the long-ranged Friedel oscillations; (ii) as we approach the Mott transition, however, these oscillations are strongly suppressed as the charge screening becomes more and more local, corresponding to a shorter “healing length”; (iii) a combination of “healing” and inelastic scattering strongly suppresses the Friedel oscillation effects even for moderate correlations.

Model and method.—We study the paramagnetic phase of the disordered Hubbard model on a cubic lattice in d

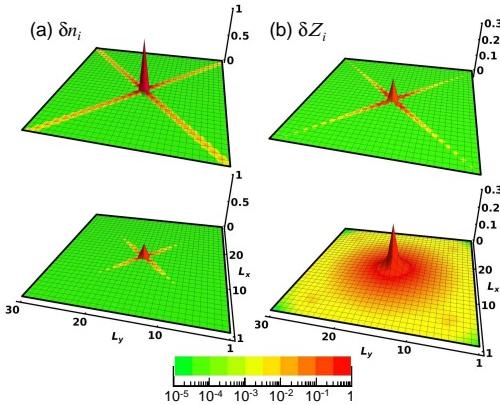


Figure 1: (a) Electronic density deviations $\delta n_i = n_i - 1$ (see text) displaying characteristic Friedel oscillations. From top to bottom we have $m/m^* = 1.00$ and 0.30 . The Friedel oscillations appear here as crosses because of the underlying Fermi surface anisotropy [7]. As we enter the strongly correlated regime, these oscillations are suppressed, similar to the “healing” effect found in Ref. [8]. (b) Quasiparticle weight deviations $\delta Z_i = Z_i - Z_0$. From top to bottom we have $m/m^* = 0.85$ and 0.08 . While for moderate values of interactions δZ_i also displays Friedel oscillations, it has a leading exponential decay close to the Mott transition. Here, we have used a 30×30 square lattice with periodic boundary conditions and $\varepsilon_o = -D$. The color scales encode only the positive values of both δn_i and δZ_i .

dimensions

$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} \varepsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where t_{ij} are the hopping matrix elements between nearest-neighbor sites, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin projection σ at site i , U is the on-site Hubbard repulsion, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator, and ε_i are the site energies. All energies will be expressed in units of the clean half-bandwidth (Fermi energy) D and we approach the Mott

metal-insulator transition (MIT) by increasing U at half filling (chemical potential $\mu = U/2$). To treat this model, we employ the slave boson mean-field theory of Kotliar and Ruckenstein [9], which is equivalent to the Gutzwiller variational approximation [10]. In this approach, the renormalized site energies v_i and the local quasiparticle weights Z_i are variationally calculated through the saddle-point solution of the corresponding Kotliar-Ruckenstein slave boson functional [11]. This theory is mathematically equivalent to a generalization of the dynamical mean field theory (DMFT) [12] to finite dimensions, the statistical DMFT (statDMFT) [13] implemented using a slave boson impurity solver [14].

At $T = 0$ and in the uniform limit ($\varepsilon_i = 0$) we have $v_0 = 0$ and $Z_0 = 1 - u^2$, with $u = U/U_c$ [9]. The critical interaction value U_c for which the Mott metal-insulator transition occurs is characterized by the divergence of the effective mass $m^* = m/Z_0$, where m is the electron band mass, indicating the transmutation of all electrons into localized magnetic moments.

We consider first a generic weak disorder potential ($|\varepsilon_i| \ll D$) and expand the resulting mean-field equations, Eqs. (5) and (6) from [14], around the uniform solution. For particle-hole symmetry $Z_i = Z_0 + O(\varepsilon_i^2)$ and, up to first order in ε_i , the renormalized disorder potential, which is the effective potential “seen” by the quasiparticles at the Fermi level, reads (summation over repeated indices implied throughout)

$$v_i = [1 - u^2]^{-1} \left(\varepsilon_i - [\mathbf{M}^{-1}(u)]_{ij} \varepsilon_j \right). \quad (2)$$

The matrix $\mathbf{M}(u)$ is the lattice Fourier transform of

$$M_{\mathbf{q}}(u) = 1 - 2g(u) \left[U_c \Pi_{\mathbf{q}}^{(0)} \right]^{-1}, \quad (3)$$

where $\Pi_{\mathbf{q}}^{(0)}$ is the usual static Lindhard polarization function [15], of the clean, non-interacting system and

$$g(u) = (1+u)(1-u)^2 [2u + u^2(1-u)]^{-1}. \quad (4)$$

Charges rearrange themselves to screen the impurity potential and the local electronic density is given by $n_i = 1 + \delta n_i$, where

$$\delta n_i = -4g(u) [U_c(1-u^2)]^{-1} [\mathbf{M}^{-1}(u)]_{ij} \varepsilon_j, \quad (5)$$

with the same spatial structure as v_i in Eq. (2).

We particularize now to a single impurity with energy ε_o placed at the site o such that $\varepsilon_i = \delta_{i,o}\varepsilon_o$. Although obtained for weak scattering, our analytical theory does capture the qualitative trends even when the scattering is not weak, as we show numerically, see Fig. (1).

Weak and strong coupling limits.— In the weak coupling regime ($u \rightarrow 0$) there is no mass renormalization and Eqs. (2) and (5) agree with the Hartree-Fock solution of the Hubbard model, with a local (static) self-energy given by $\Sigma_i = Un_i^0$, where $n_i^0 = 1 + 2\Pi_{ij}^{(0)}\varepsilon_j$ is

the non-interacting electronic density and $\Pi_{ij}^{(0)}$ is the lattice Fourier transform of $\Pi_{\mathbf{q}}^{(0)}$. Even though the bare impurity potential ε_i is localized in space, the density deviation δn_i^0 displays long-ranged Friedel oscillations encoded in $\Pi_{ij}^{(0)}$. For example, in a free electron gas we have $\delta n(r) \sim \cos(2k_F r)/r^d$, where r is the distance to the impurity and k_F is the Fermi momentum. Slowly decaying Friedel oscillations are a direct consequence of the gapless nature of Fermi liquid excitations. The renormalized disorder potential reads $v_i \simeq \varepsilon_i + U\Pi_{ij}^{(0)}\varepsilon_j$, implying that the electrons scatter not only off the local bare impurity, but also off the long-ranged potential generated by the Friedel oscillations.

As we approach the critical region ($u \rightarrow 1$), however, the density deviation in Eq. (5) becomes

$$\delta n_i = -\frac{2(1-u)}{U_c} \left[\varepsilon_i + \frac{2}{U_c} (1-u)^2 [\mathbf{\Pi}^{(0)}]_{ij}^{-1} \varepsilon_j \right], \quad (6)$$

showing a suppression of the Friedel oscillations: the non-local part of δn_i is a factor $(1-u)^2$ smaller than the local one. Therefore, the electronic density is significantly disturbed only in the vicinity of the impurities, implying a much shorter “healing length”, see Fig. (1)(a). The suppression of the slow spatial decay in δn_i reflects the fundamental tendency of quasiparticles to become localized as the system approaches the Mott insulator.

The renormalized disorder potential, Eq. (2), is

$$v_i = -(1-u) U_c^{-1} [\mathbf{\Pi}^{(0)}]_{ij}^{-1} \varepsilon_j, \quad (7)$$

and the screened impurity potential is just as non-local as for small u , except for a reduction of the overall amplitude scale. Therefore, we should not be guided by density fluctuations alone which are indeed healed very effectively. However, we notice that v_i goes to zero linearly at all lattice sites at the transition, signaling a complete suppression of disorder by interactions [16].

To obtain the leading energy correction of Z_i , we have to expand the mean-field equations up to second order in ε_i . At intermediate values of the interaction, deviations in the quasiparticle weights $\delta Z_i = Z_i - Z_0$ also show Friedel-like oscillations. Close to the Mott transition, δZ_i displays a leading exponential decay from the impurity site, since all additional terms describing its long-range oscillations are of higher order in $(1-u)$, see Fig. (1)(b) and Eq. (8) below (the details of the calculation will be presented elsewhere). A finite impurity potential tends to push the site occupation away from half filling, thus reducing the tendency to form a local moment and rendering the given site locally more metallic by increasing Z_i . As spatial correlations grow, this “metallization” of the correlated metal tends to spread out away from the impurity, thus creating metallic “puddles” (red region in Fig. (1)(b)) in an almost-localized host. A somewhat similar result emerges in the $t-t'-J$ model, in which

an impurity induces a local staggered magnetization in its vicinity [17, 18] whose spatial extent also increases with correlations. The critical behavior of δZ_i is captured by our analytical expressions and we can show that, for $d \geq 2$, and $r_{io}/\xi \gg 1$

$$\begin{aligned} \delta Z_i &\sim \frac{1-u}{U_c^2} \left(\frac{\pi^{(1-d)/2}}{2^{(1+d)/2} \xi^{(d-3)/2}} e^{-r_{io}/\xi} \right. \\ &\quad \left. - 4(1-u)^3 [\Pi^{(0)}]_{io}^{-1} \right) \varepsilon_o^2 \end{aligned} \quad (8)$$

where $r_{io} = |\mathbf{r}_i - \mathbf{r}_o|$, z is the coordination number, and $\xi = (2z(1-u))^{-1/2}$ plays the role of a correlation length. This correlation length diverges at the transition with a mean field exponent 1/2. Previous studies on the interface of a strongly correlated metal and a Mott insulator [19, 20], which use techniques similar to ours, also find an analogous leading exponential decay of the quasiparticle weight upon entering the Mott insulator from the metal. In those studies, however, the oscillating terms of Eq. (8) seem to have been overlooked.

Leading finite T corrections for transport and inelastic cutoffs.—We would like now to go beyond $T = 0$ and study the behavior of the leading temperature corrections to the resistivity $\rho(T)$ as a function of the correlations. We focus henceforth only on $2d$ systems, since, in the weakly correlated regime, electron scattering by Friedel oscillations leads to a non-Fermi-liquid linear temperature correction to $\rho(T)$ [6, 21] in the ballistic regime.

The transport scattering rate is given by

$$\tau_{\text{tr}}^{-1}(\varepsilon) = n_{imp} m \int_0^{2\pi} \frac{d\theta}{2\pi} |T_q|^2 (1 - \cos\theta), \quad (9)$$

where n_{imp} is the impurity concentration, T_q is the Fourier transform of the T matrix, $q = 2k\sin\theta/2$ is the transferred momentum, θ is the scattering angle. To simplify our analytical expressions, we henceforth focus on the case a free electron dispersion $\varepsilon = k^2/2m$; we carefully checked that no significant changes are found if a different dispersion is used. Up to first order in the impurity potential ε_o , the T matrix is simply given by the renormalized disorder potential v_i (Eq. (2)). The scattering time is given by the average $\tau_{\text{tr}} = \int d\varepsilon \tau_{\text{tr}}(\varepsilon) f'(\varepsilon)$, where $f'(\varepsilon)$ is the derivative of the Fermi distribution function.

In our slave boson mean-field theory, the electronic self-energy is purely real [9] and describes only the elastic scattering of the electrons off a temperature dependent screened impurity potential. However, this scheme should really be regarded as a variational calculation of the quasiparticle parameters within our statDMFT procedure. In a fuller treatment, there is also an imaginary part in the self-energy, reflecting inelastic effects. For the purposes of examining the *leading perturbative effects* of impurity scattering, the imaginary part can be computed in the uniform system, where it emerges naturally in the

context of local Fermi liquid theories like DMFT [12, 22] and is given by

$$\gamma(T) = \Lambda(u) T_F (T/T_F)^2, \quad (10)$$

where T_F is the Fermi temperature and the function $\Lambda(u)$ has the following limits: $\Lambda(u) \sim u^2$ for small u and $\Lambda(u) \sim (1-u)^{-2} \sim (m^*/m)^2$ close to the Mott transition. These limits can be understood from the fact that in the weakly correlated regime inelastic scattering effects are perturbative, whereas in the strongly correlated regime we recover the well known Kadowaki-Woods relation [22], observed in several strongly correlated systems, and which holds within the DMFT picture we use.

There are two leading contributions from inelastic scattering. A bulk one, present even in the clean limit, given by $\tau_{in}^{-1}(T) = \eta \gamma(T)$, where η is a geometrical factor depending on the band structure used in the DMFT calculation. $\tau_{in}^{-1}(T)$ simply adds to $\tau_{\text{tr}}^{-1}(T)$ in Eq. (9) through Matthiessen's rule, since we consider very dilute impurities. In addition to this, a finite imaginary part also *cuts off the leading non-analyticities of the elastic scattering off Friedel oscillations* [6, 23]. This is taken into account in the calculation of $\Pi_{\mathbf{q}}^{(0)}$, considering that the electron energy has now an imaginary part given by $\gamma(T)$. The calculation of $\Pi_{\mathbf{q}}^{(0)}$ in the presence of inelastic broadening is carefully discussed in Ref. [23] for the $2d$ electron gas and we use the analytical form of $\Pi_{\mathbf{q}}^{(0)}$ as obtained there.

The final form of $\tau_{\text{tr}}^{-1}(T)$, valid for $T \ll T_F$, reads

$$\begin{aligned} \tau_{\text{tr}}^{-1}(T) &= \tau_0^{-1} A^2(u) \left\{ 1 + 2 \frac{T}{T_F} \alpha(u) w(T, \gamma(T)) \right\} \\ &\quad + \eta \gamma(T), \end{aligned} \quad (11)$$

where

$$\begin{aligned} w(T, \gamma) &= \int_{-\infty}^{+\infty} \frac{dx}{4} \operatorname{sech}^2\left(\frac{x}{2}\right) \operatorname{Re} \left[\ln \Gamma \left(\frac{2\pi}{\pi + \frac{\gamma(T)}{T} + ix} \right) \right] \\ &\quad + \frac{1}{2} \ln(2\pi) + \frac{\gamma(T)}{2\pi T} \ln \left(\frac{T_F}{2\pi T} \right), \end{aligned} \quad (12)$$

$$A(u) = g(u) [(1-u^2)(\rho(\varepsilon_F) U_c + g(u))]^{-1}, \quad (13)$$

$$\alpha(u) = 2\rho(\varepsilon_F) U_c [\rho(\varepsilon_F) U_c + g(u)]^{-1}, \quad (14)$$

τ_0^{-1} is the zero-temperature impurity scattering rate, $\rho(\varepsilon_F)$ is the clean electronic density of states at the Fermi level and $\Gamma(z)$ is the Gamma function. The function $A(u)$ controls the amplitude of the scattering rate from the screened impurity potential. In the weakly interacting regime $A(u) \sim 1$, whereas in the critical region $A(u) \sim (1-u)$ due to a vanishing v_i at $U = U_c$, Eq. (7). The function $\alpha(u)$ gives the strength of the leading temperature correction. It goes as U for weak correlations,

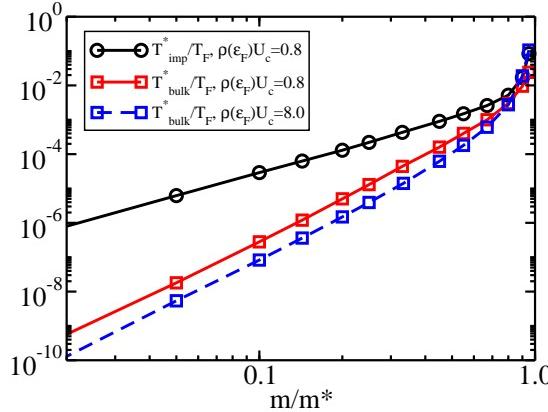


Figure 2: Limiting temperatures to the linear in T regime of the resistivity of a $2d$ electron liquid on a log-log scale, calculated under two different assumptions (see text) for two values of the parameter $\rho(\epsilon_F)U_c$ [24]. T_{imp}^* is almost independent of $\rho(\epsilon_F)U_c$ and only one curve is shown here. T_{bulk}^* is the dominating cutoff above which the linear behavior is lost. Here, we have used $\tau_0\epsilon_F = 10$, corresponding to a weak impurity potential.

indicating that the temperature corrections only arise in the presence of electron-electron repulsion, and saturates to 2 close to the Mott transition. The function $w(T, \gamma)$ encodes the dependence of the leading temperature correction on $\gamma(T)$.

For $\gamma(T) = 0$, only elastic scattering is present and we obtain $w(T, 0) = 0.5$. Plugging this into Eq. (11), we see that the linear in T correction is found for all $u > 0$ [6] and is limited only by the overall amplitude $A(u)$, which is in accordance with Eq. (7).

However, for a finite $\gamma(T)$, the linear region of $\rho(T)$ considerably narrows as we enter the correlated regime. As there are two leading contributions from inelastic scattering, we analyze their individual effects separately by defining two threshold temperatures bounding the non-Fermi-liquid region from above. They are obtained by comparing the purely elastic $\tau_{tr}^{-1}(T)$ ($\gamma(T) \rightarrow 0$ in Eq. (11)) with two other scattering rates: one in which we let $\eta \rightarrow 0$ (T_{imp}^*) and the other in which we set $w(T, \gamma) \rightarrow w(T, 0)$ (T_{bulk}^*) in Eq. (11). We interpolate the function $\Lambda(u)$ using DMFT with both quantum Monte Carlo and iterated perturbation theory [25] as impurity solvers. We use $\eta = 10$, a value also in agreement with DMFT calculations [25]. As we can see from Fig. (2), T_{bulk}^* is strictly smaller than T_{imp}^* . This is because T_{bulk}^* is not only proportional to the infinitesimal impurity concentration n_{imp} (or, equivalently, to $(\tau_0\epsilon_F)^{-1}$) but, in the critical region, $T_{bulk}^* \sim (m/m^*)^4$, whereas $T_{imp}^* \sim (m/m^*)^2$. Thus, for any degree of correlations, it is T_{bulk}^* which sets the upper bound on the linear in T region of $\rho(T)$. From Fig. (2) we see that, even for very moderate correlations, e.g. for $m/m^* \sim 0.9$, $T_{bulk}^* \sim 10^{-2}T_F$, and for $m/m^* \sim 0.6$, already $T_{bulk}^* \sim 10^{-4}T_F$. Thus, the non-

Fermi liquid region is limited to very low temperatures. Ultimately, as the linear in T regime is also bounded from below by a crossover to the diffusive regime, the ballistic T -interval in which these elastic corrections dominate may not be present at all.

Conclusions.—We presented a detailed, mostly analytical, model calculation of the effects of a single non-magnetic impurity placed in a correlated host. We find that strong correlations tend to reduce the effects of the long-range part of the Friedel oscillations and our work provides clear analytical insight into how this happen. It should be possible to directly test our quantitative predictions by means of current generation scanning tunneling microscopy methods, shedding new light on the behavior near the Mott MIT. It is noteworthy that impurities placed in d-wave superconductors also produce slowly decaying perturbations in real space, reflecting their gapless nature, through a mechanism closely related to Friedel oscillations in normal metals. Recent work by Garg *et al.* [8] shows, by using a very similar theoretical approach as we do, that in this system strong correlations also lead to spatial “healing”. We believe that both phenomena have a closely related origin and our results strongly suggest that the “healing” effect is a more general property of correlated metals close to the Mott transition, not an effect specific to cuprates or the superconducting state.

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